Mixing MARTINI

Wassenaar, Tsjerk A.; Ingólfsson, Helgi I.; Priess, Marten; Marrink, Siewert J.; Schaefer, Lars V.

Published in:
Journal of Physical Chemistry B

DOI:
10.1021/jp311533p

Mixing Martini: Electrostatic Coupling in Hybrid Atomistic – Coarse-Grained Biomolecular Simulations

*Tsjerk A. Wassenaar[$,§], Helgi I. Ingólfsson[$,§], Marten Prieß[#], Siewert J. Marrink[$], and Lars V. Schäfer[#,]**

[$]Groningen Biomolecular Sciences and Biotechnology Institute & Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 7, 9747 AG Groningen, The Netherlands

[#]Institute of Physical and Theoretical Chemistry, Goethe University Frankfurt, Max-von-Laue-Str. 7, D-60438 Frankfurt am Main, Germany

*email: schaefer@chemie.uni-frankfurt.de

§ These authors contributed equally to this work.

Table S1. Maxima and minima of the PMFs. Local maxima and minima are given in *italic*.

	d (nm)	ΔG (kJ/mol)	d (nm)	ΔG (kJ/mol)
Na+/Cl-				
SPC/E	0.25	-8.2	0.35	5.3
PW (CG)	0.46	-9.1	0.67	0.1
BMW (CG)	0.46	-9.5	2.11	0.1
NaCl(0) PW	0.31	-6.2	0.66	3.1
PW 1.0	*0.23*	*193.3*	*0.36*	*227.5*
PW 1.1	*0.23*	*83.0*	*0.41*	*147.4*
PW 1.25	0.23	-33.6	0.47	73.9
PW 1.3	0.24	-57.4	0.48	57.7
PW 1.45	0.23	-137.3	0.56	21.5
PW 1.5	0.23	-155.4	0.57	13.5
PW 2	0.26	-271.6		
BMW 1.0	0.23	-93.2	0.50	38.9
BMW 1.1	0.23	-150.3	0.56	14.3
BMW 1.2	0.23	-195.9	2.16	0.0
BMW 1.3	0.23	-231.8	2.04	0.1
BMW PME	0.46	-7.9	0.65	0.8
PW PME	0.46	-7.2	0.67	1.9
Lys/Glu				
SPC/E	*0.53*	*-3.2*	*0.65*	*-2.8*
	0.92	-3.3	2.05	0.0
PW (CG)	*0.46*	*-5.2*	*0.75*	*-0.7*
	0.94	-2.7	2.08	0.1
BMW (CG)	*0.46*	*-2.7*	*0.71*	*-1.7*
	0.92	-4.2	2.05	-0.1
Std CG water ε=15	0.47	-11.0	2.12	0.1
Std CG water ε=78	0.50	-2.6	0.76	1.4
PW ε=1.0	1.34	-7.8		
PW ε=1.45	0.44	-8.7	0.65	5.0
PW ε=1.5	0.44	-20.7		
BMW ε=1.0	*1.00*	*-1.4*	*1.15*	*-0.8*
	1.40	-1.8	1.99	0.3
BMW ε=1.1	0.46	-8.7	0.66	4.8
BMW ε=1.15	0.46	-30.6	0.71	0.2
BDW ε=2.3	0.49	-156.2		
Glu/Glu				
SPC/E 2Na+	*0.64*	*3.2*	*0.74*	*3.7*
	0.91	*2.7*	*0.97*	*2.7*
	2.03	-0.1	2.16	0.0
SPC/E no counterions	*0.65*	*5.5*	*0.73*	*5.7*
	0.92	4.5	0.94	4.5
PW (CG)	1.80	-0.2	2.08	0.0
BMW (CG)	0.91	2.9	1.06	3.5
PW ε=1.45 2Na+	*0.51*	*-3.9*	*0.65*	*-1.6*
	0.79	-4.3	1.09	3.4
PW ε=1.45 no counterions	0.50	0.7	*0.70*	*4.9*
	0.82	*3.9*	1.09	6.2
PW ε=1.75 2Na+	1.82	0.2	1.96	0.4
BMW 1.1 2Na+	0.80	-3.5	1.08	2.8
BMW 1.1 no counterions	0.80	-0.9	1.06	4.6
Ser/Ser				
SPC/E	0.44	-1.0	0.61	0.8
PW (CG)	0.52	-2.0	0.73	2.2
BMW (CG)	0.94	-1.7	1.21	1.2

Std CG water	0.33	-22.2	0.69	2.6
PW ε=1.0	0.32	-20.4	0.67	3.3
PW ε=1.45	0.33	-20.3	0.68	2.8
PW/s ε=1.45	0.33	-16.0	0.61	1.8
BMW ε=1.1	0.32	-15.3	0.59	4.9
BMW/s ε=1.1	0.33	-10.2	0.54	3.2
BDW ε=2.3	0.33	-3.8	0.41	0.9
NMA/NMA				
SPC/E	0.45	-3.0	1.95	0.0
Std CG water	0.45	-20.3	1.17	0.3
PW ε=1.0	0.38	-9.4	0.68	0.2
PW ε=1.45	0.44	-10.9	0.74	1.2
BMW ε=1.1	0.44	-6.7	1.75	0.4
BDW ε=2.3	0.46	-3.5	1.57	0.1
Phe/Phe				
SPC/E	0.53	-2.8	0.82	0.4
PW (CG)	0.57	-6.4	0.90	1.6
BMW (CG)	*0.68*	*-2.0*	*0.82*	*-0.5*
	1.03	-2.6	1.36	0.6
Std CG water	0.51	-4.3	0.85	2.2
PW ε=1.45	0.52	-3.6	0.85	2.0
BMW ε=1.0	*0.65*	*2.3*	*0.75*	*2.6*
	1.03	-1.3	1.32	1.5
BMW ε=1.1	*0.63*	*2.7*	*0.74*	*3.0*
	1.04	-1.4	1.34	1.4
BDW ε=2.3	0.56	-1.7	0.85	0.3
Val/Val				
SPC/E	0.49	-2.0	0.68	1.0
PW (CG)	0.51	-5.5	1.17	0.4
BMW (CG)	*0.55*	*1.0*	*0.65*	*2.2*
	0.91	-0.5	1.19	1.9
PW	0.45	-6.0	0.76	0.6
BMW	*0.46*	*-0.7*	*0.66*	*1.5*
	0.92	-1.5	1.21	1.0
Std CG water	0.45	-6.5	1.18	0.3
BDW	0.52	-2.1	0.79	0.8